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FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26  
FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L100 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:241344 HCAPLUS  
DN 136:279199  
TI Preparation of phenolic and thiophenolic ethers and their derivs. as  
cytosolic **phospholipase A2** inhibitors  
IN Banville, Jacques; Remillard, Roger;  
Balasubramanian, Neelakantan; Bouthillier, Gilles;  
Martel, Alain  
PA Can.  
SO U.S. Pat. Appl. Publ., 71 pp.  
CODEN: USXXCO  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002037875	A1	20020328	US 2001-848694	20010503 <--
PRAI	US 2000-203741P	P	20000511 <--		
OS	MARPAT 136:279199				
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I (X = O, S(O)n, (un)substituted amine, amide or -CH2- with provision when X = -CH2-, R1 and R2 = halo; n = 0-2; X1 = H, CF3, OCF3, halo, (un)substituted alkyl, alkenyl, alkynyl or cycloalkyl; Z = OR6, S(O)nR6, NR6R7 or CHR6R7; R1 and R2 = H, halo, (un)substituted alkoxy, cycloalkyloxy, alkyl, etc.; Ra and Rb may together form oxo group or independently = H, OH, NH2, N3, F, etc.; R3, R4 and R5 independently = H, halo, (un)substituted alkoxy, alkenyloxy, alkyl, alkenyl, etc.; R6 and R7 independently = H, (un)substituted alkyl, alkenyl, alkynyl, aryl, silyl, etc.) are prepared and disclosed as **phospholipase** inhibitors. Thus, II was prepared in six steps from 1,2-epoxy-3-[4-(tert-butoxycarbonyl)phenoxy]propane and 3-(4-hydroxyphenyl)-1-(tert-

butyldiphenylsilyloxy)propane with the final step prior to hydrolysis of a protected intermediate ester being substitution of 3-[4-(3-methanesulfonyloxypropyl)phenoxy]-1-[4-(tert-butoxycarbonyl)phenoxy]-2-propanone with N-methyl-2-bis-(4-chlorophenyl)ethylamine. As inhibitors of the cytosolic **phospholipase A2** enzymes, I are useful in controlling a wide variety of inflammatory diseases (no data).

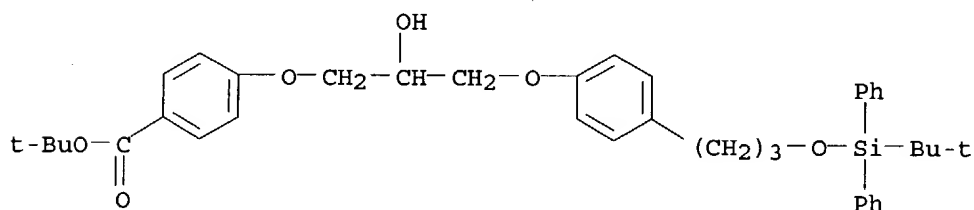
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 405553-74-4P 405553-75-5P 405553-76-6P  
 405553-77-7P 405553-78-8P 405553-79-9P  
 405553-87-9P 405553-92-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of phenolic and thiophenolic ethers and their derivs. as cytosolic **phospholipase A2** inhibitors)

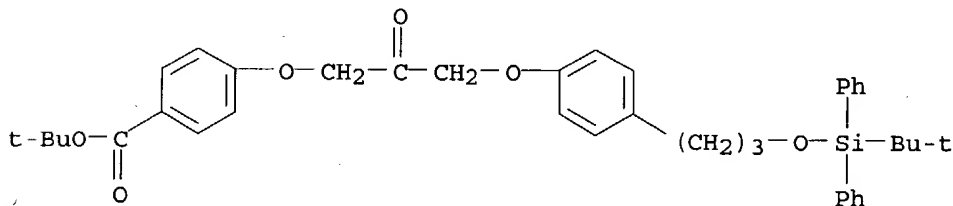
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CN Benzoic acid, 4-[3-[4-[3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]propyl]phenoxy]-2-hydroxypropoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



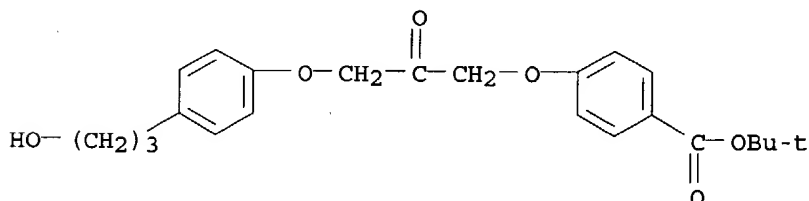
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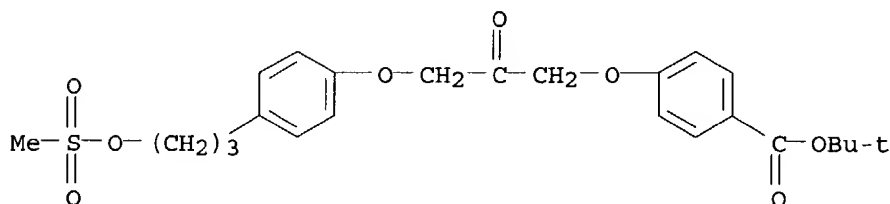
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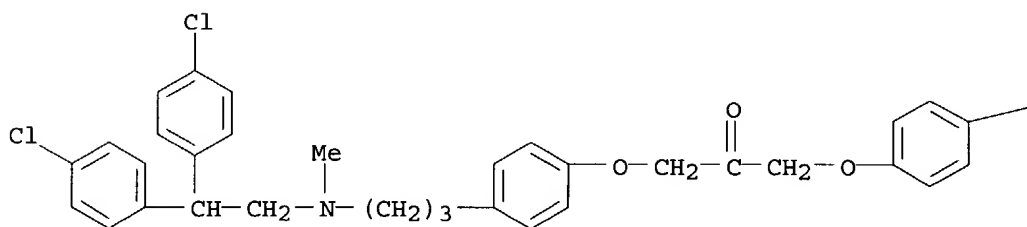
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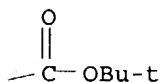
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CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-oxopropoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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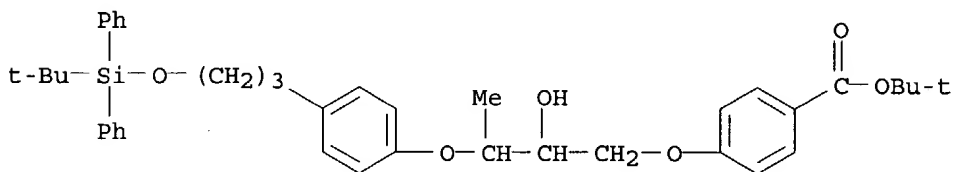


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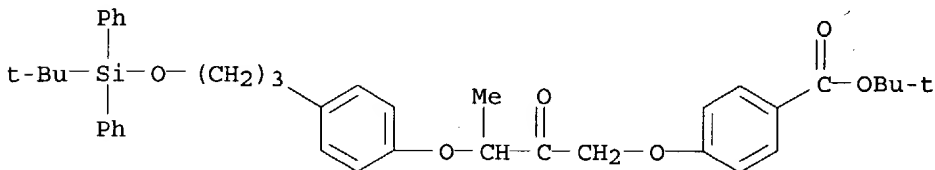
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CN Benzoic acid, 4-[3-[4-[3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]propyl]phenoxy]-2-hydroxybutoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



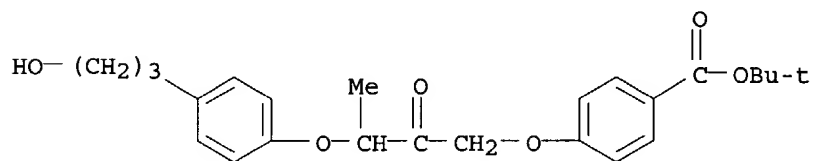
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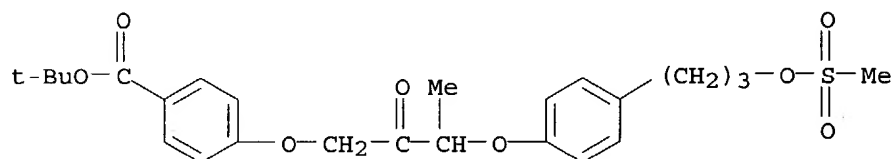
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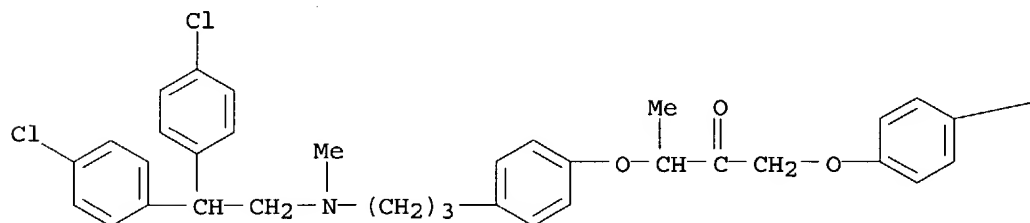
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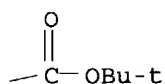
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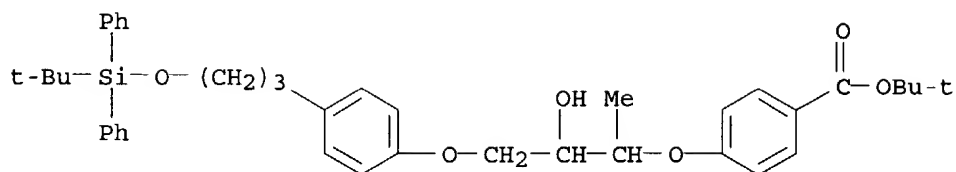


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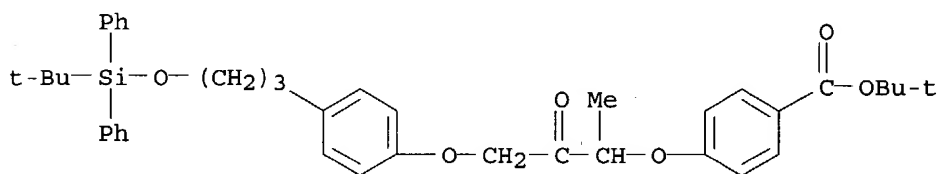
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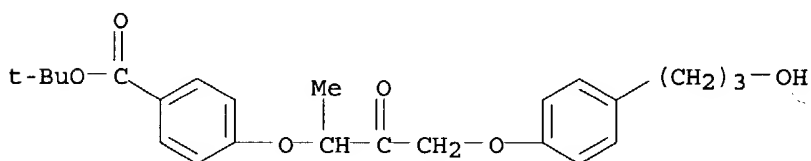
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CN Benzoic acid, 4-[3-[4-[3-[(1,1-dimethylethyl)diphenylsilyl]oxy]propyl]phenoxy]-1-methyl-2-oxopropoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



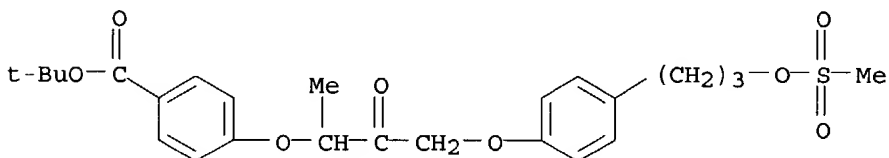
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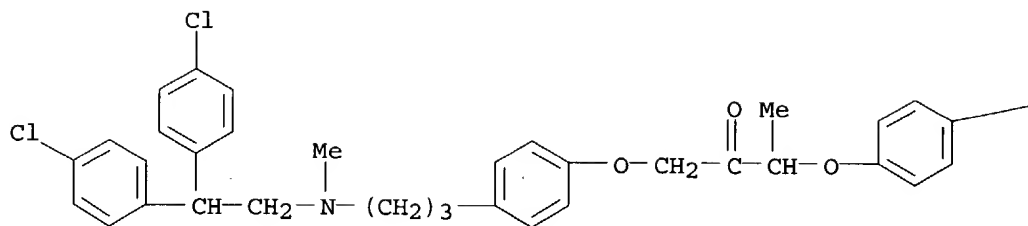
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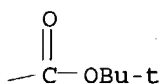
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CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-1-methyl-2-oxopropoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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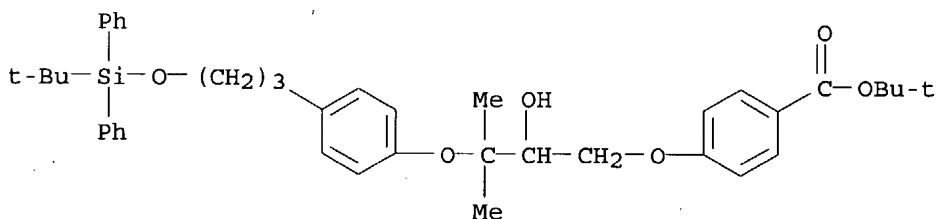


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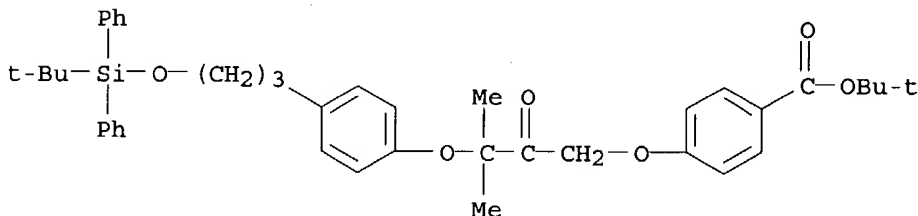
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CN Benzoic acid, 4-[3-[4-[3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]propyl]phenoxy]-2-hydroxy-3-methylbutoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



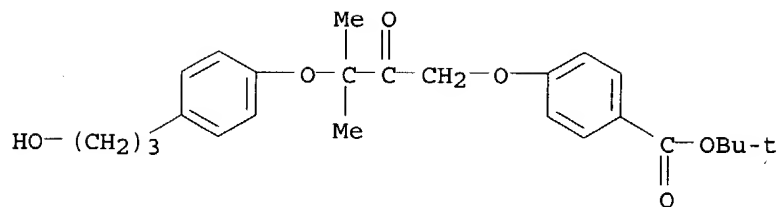
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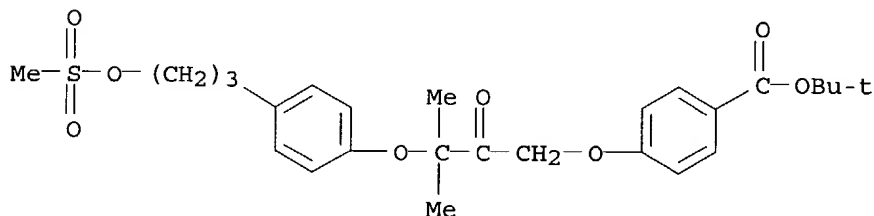
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RN 405553-71-1 HCAPLUS

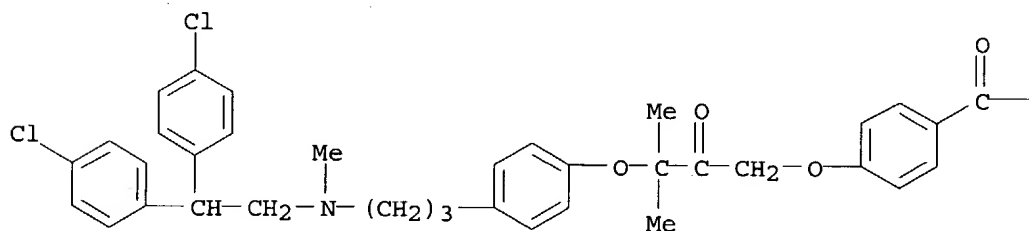
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RN 405553-72-2 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-3-methyl-2-oxobutoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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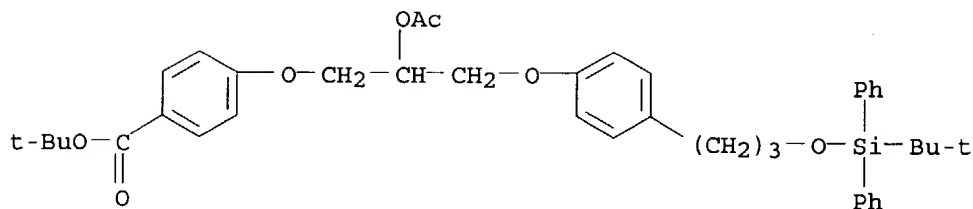


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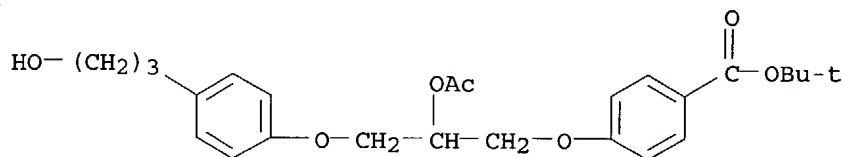
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CN Benzoic acid, 4-[2-(acetyloxy)-3-[4-[3-[[1,1-dimethylethyl]diphenylsilyl]oxy]propyl]phenoxy]propoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



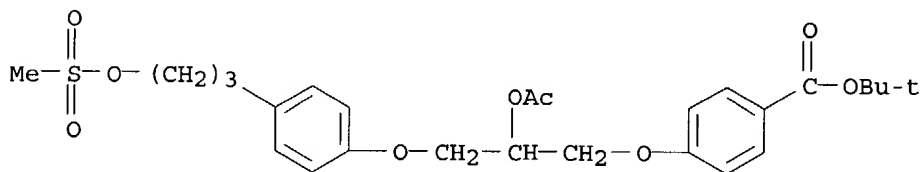
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CN Benzoic acid, 4-[2-(acetyloxy)-3-[4-(3-hydroxypropyl)phenoxy]propoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



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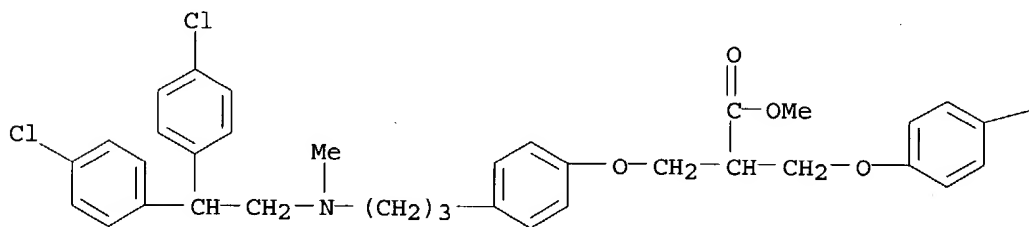
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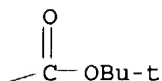
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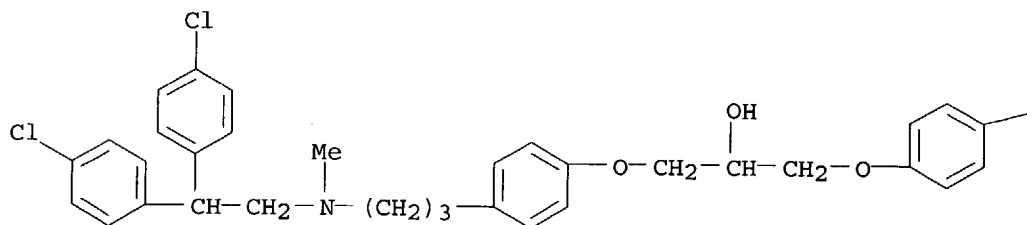


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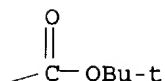


CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-hydroxypropoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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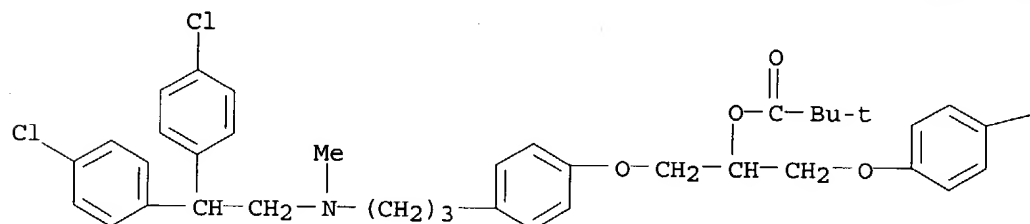
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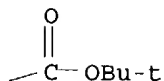
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CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-(2,2-dimethyl-1-oxopropoxy)propoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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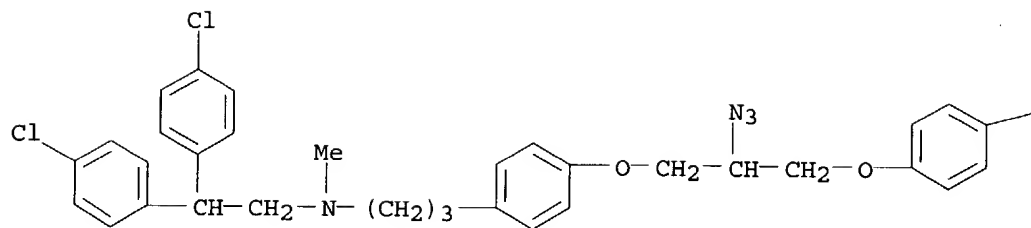
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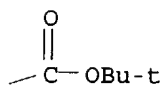
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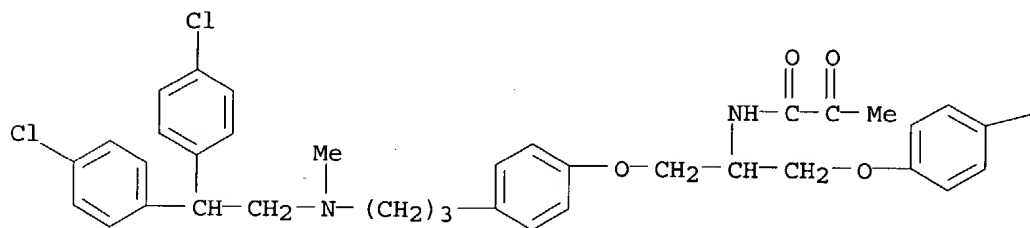
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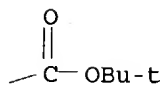
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(9CI) (CA INDEX NAME)

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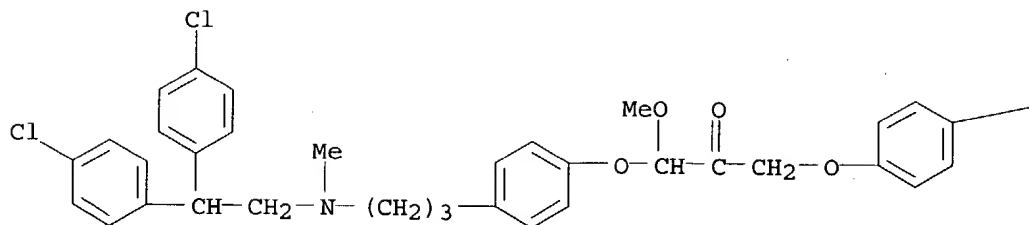
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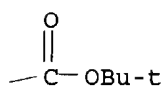
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CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]  
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INDEX NAME)

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IT 405552-77-4P 405552-79-6P 405552-83-2P  
 405552-87-6P 405552-92-3P 405552-95-6P  
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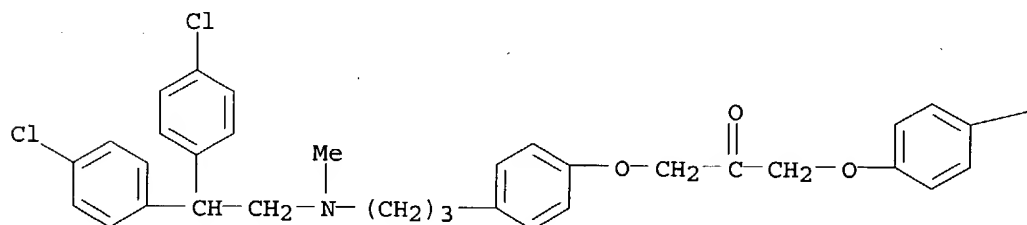
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(target compound; preparation of phenolic and thiophenolic ethers and their derivs. as cytosolic **phospholipase** A2 inhibitors)

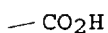
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CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-oxopropoxy]- (9CI) (CA INDEX NAME)

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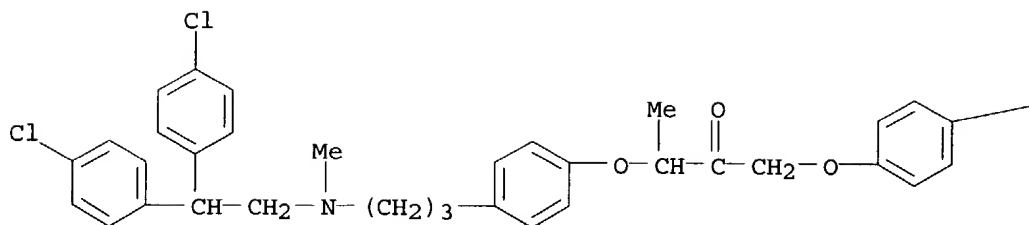
PAGE 1-B



RN 405552-79-6 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-oxobutoxy]- (9CI) (CA INDEX NAME)

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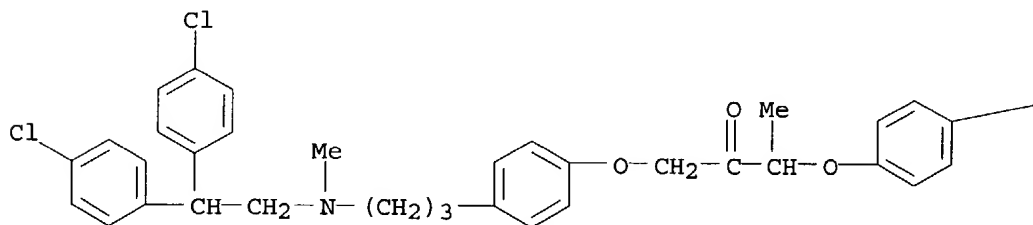
PAGE 1-B

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CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-1-methyl-2-oxopropoxy]-(9CI) (CA INDEX NAME)

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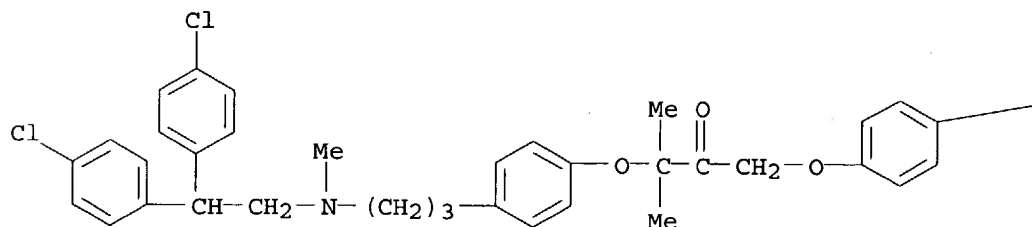
PAGE 1-B

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RN 405552-87-6 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-3-methyl-2-oxobutoxy]-(9CI) (CA INDEX NAME)

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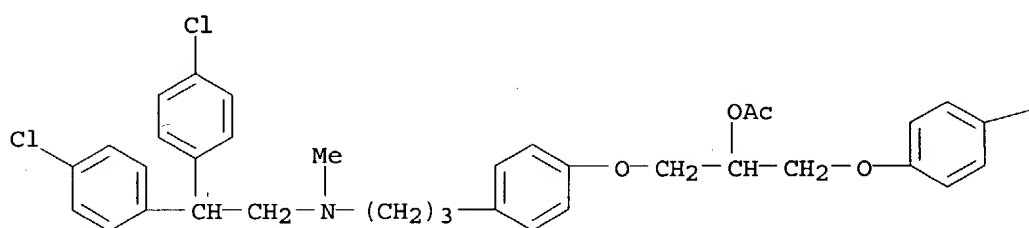
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RN 405552-92-3 HCAPLUS

CN Benzoic acid, 4-[2-(acetyloxy)-3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]propoxy]-(9CI) (CA INDEX NAME)

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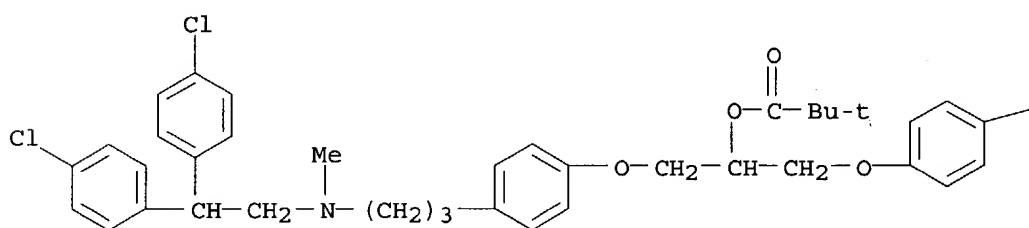
PAGE 1-B

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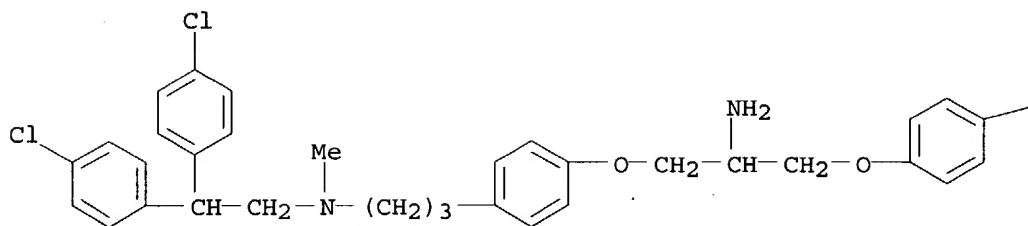
PAGE 1-B

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RN 405552-98-9 HCAPLUS

CN Benzoic acid, 4-[2-amino-3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]propoxy]-(9CI) (CA INDEX NAME)

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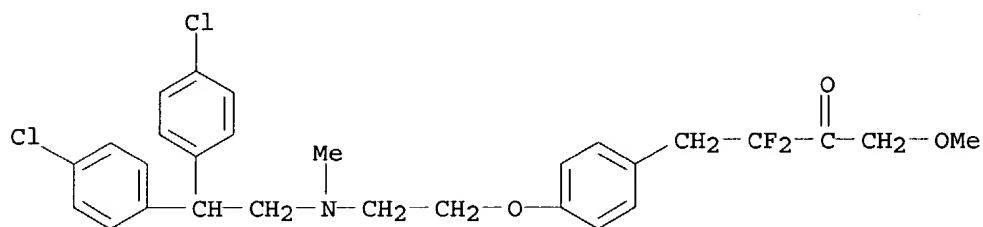


PAGE 1-B

-CO<sub>2</sub>H

RN 405553-00-6 HCAPLUS

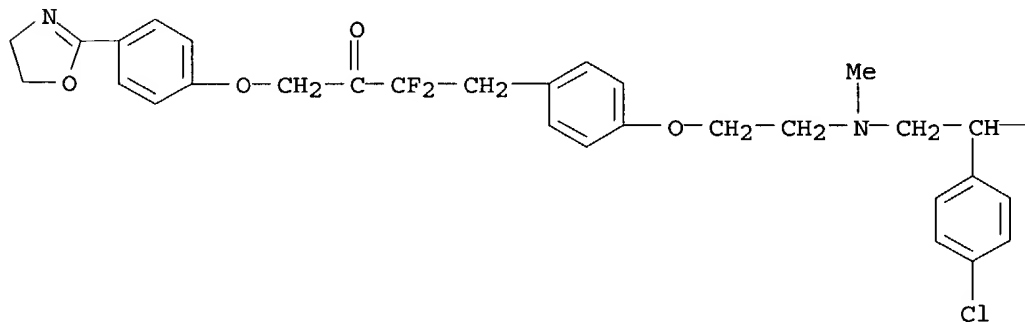
CN 2-Butanone, 4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-3,3-difluoro-1-methoxy- (9CI) (CA INDEX NAME)



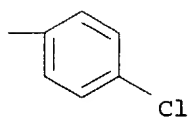
RN 405553-02-8 HCAPLUS

CN 2-Butanone, 4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-1-[4-(4,5-dihydro-2-oxazolyl)phenoxy]-3,3-difluoro- (9CI) (CA INDEX NAME)

PAGE 1-A

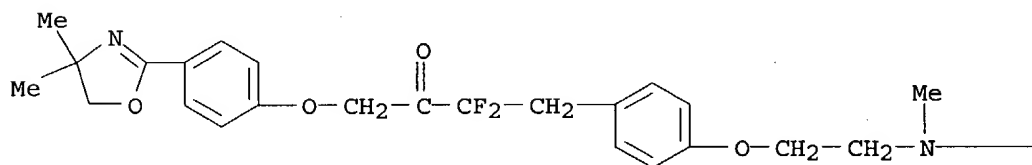


PAGE 1-B

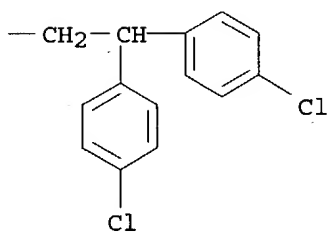


RN 405553-04-0 HCAPLUS  
 CN 2-Butanone, 4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-1-[4-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)phenoxy]-3,3-difluoro- (9CI)  
 (CA INDEX NAME)

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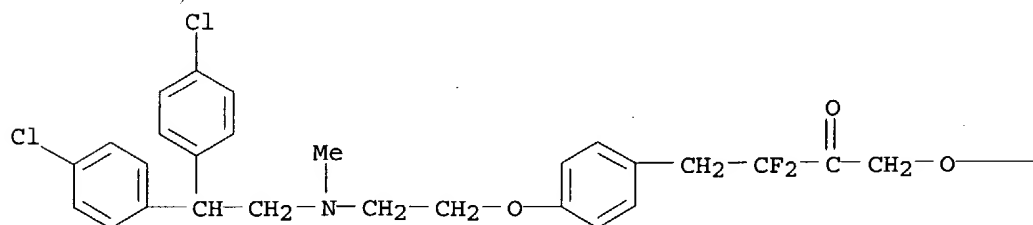


PAGE 1-B

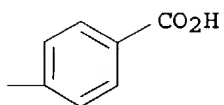


RN 405553-07-3 HCAPLUS  
 CN Benzoic acid, 4-[4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-3,3-difluoro-2-oxobutoxy]- (9CI) (CA INDEX NAME)

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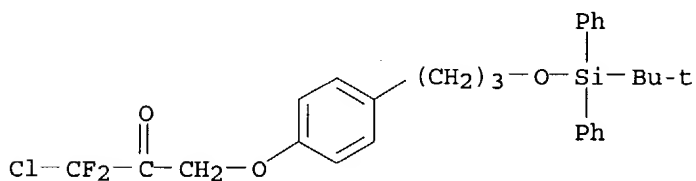
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 405553-06-2P 405553-09-5P 405553-11-9P  
 405553-12-0P 405553-13-1P 405553-14-2P  
 405553-15-3P 405553-17-5P 405553-19-7P  
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 405553-26-6P 405553-27-7P 405553-28-8P  
 405553-29-9P 405553-31-3P 405553-32-4P  
 405553-33-5P 405553-34-6P 405553-35-7P  
 405553-36-8P 405553-37-9P 405553-38-0P  
 405553-39-1P 405553-40-4P 405553-41-5P  
 405553-42-6P 405553-43-7P 405553-44-8P  
 405553-45-9P 405554-14-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of phenolic and thiophenolic ethers and their derivs. as cytosolic **phospholipase A2** inhibitors)

RN 405552-74-1 HCAPLUS

CN 2-Propanone, 1-chloro-3-[4-[3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]propyl]phenoxy]-1,1-difluoro- (9CI) (CA INDEX NAME)

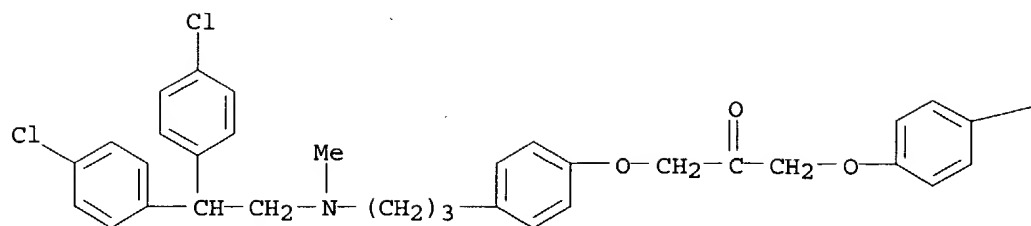


RN 405552-78-5 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-oxopropoxy]-, hydrochloride (9CI) (CA INDEX NAME)



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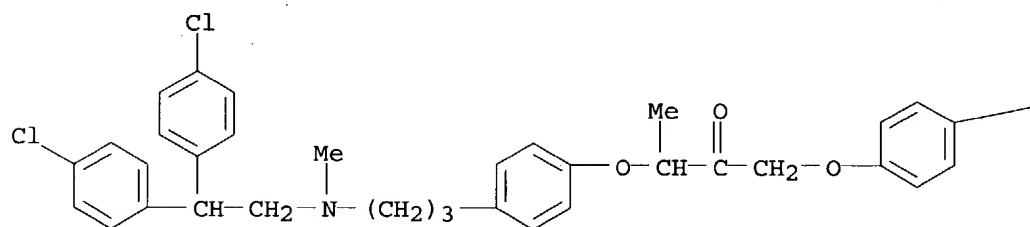
● HCl

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—CO<sub>2</sub>H

RN 405552-80-9 HCAPLUS  
 CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-oxobutoxy]-, hydrochloride (9CI) (CA INDEX NAME)

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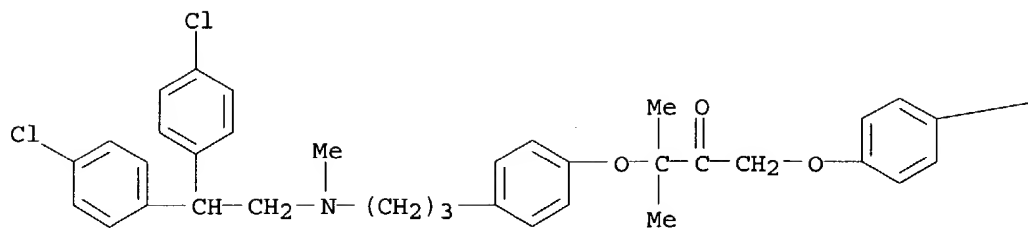
● HCl

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—CO<sub>2</sub>H

RN 405552-90-1 HCAPLUS  
 CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-3-methyl-2-oxobutoxy]-, hydrochloride (9CI) (CA INDEX NAME)

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● HCl

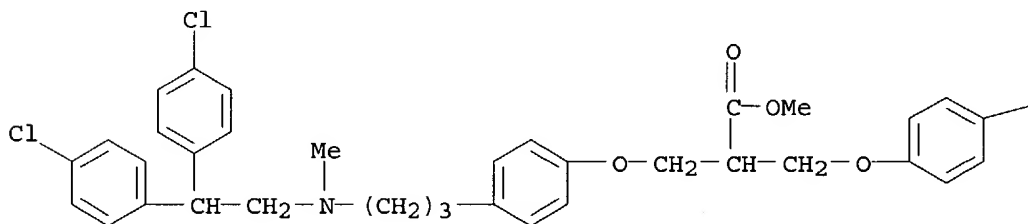
PAGE 1-B

—CO<sub>2</sub>H

RN 405552-93-4 HCAPLUS

CN Benzoic acid, 4-[2-[[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]methyl]-3-methoxy-3-oxopropoxy]-, hydrochloride (9CI) (CA INDEX NAME)

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● HCl

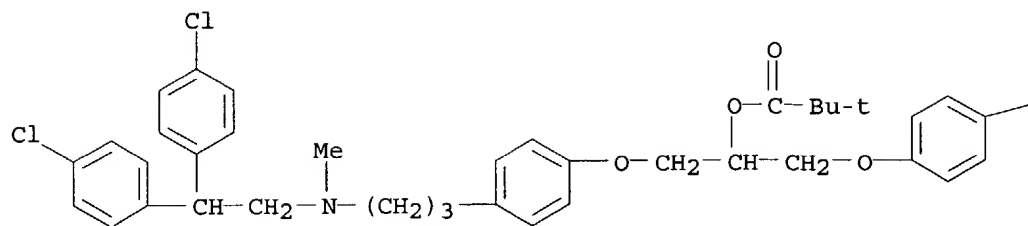
PAGE 1-B

—CO<sub>2</sub>H

RN 405552-97-8 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-(2,2-dimethyl-1-oxopropoxy)propoxy]-, hydrochloride (9CI) (CA INDEX NAME)

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● HCl

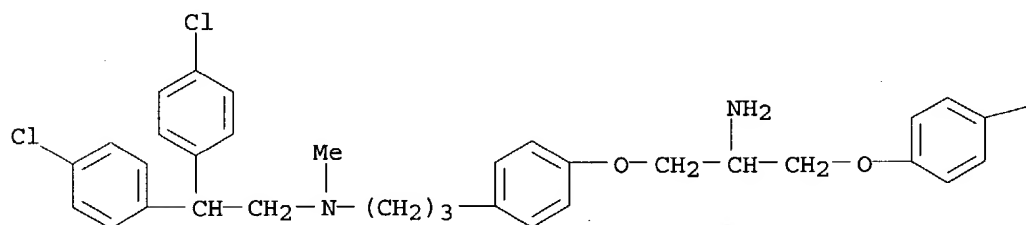
PAGE 1-B

—CO<sub>2</sub>H

RN 405552-99-0 HCAPLUS

CN Benzoic acid, 4-[2-amino-3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamin  
o]propyl]phenoxy]propoxy]-, dihydrochloride (9CI) (CA INDEX NAME)

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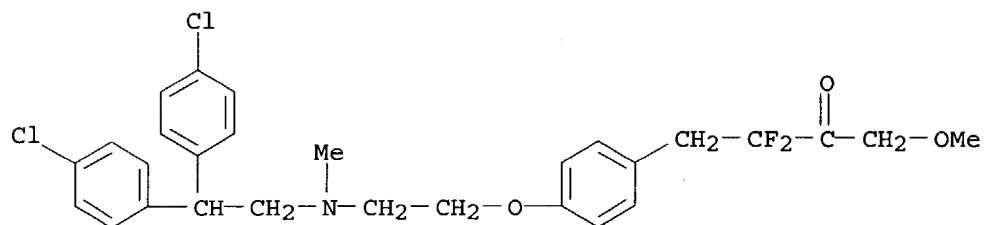
● 2 HCl

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—CO<sub>2</sub>H

RN 405553-01-7 HCAPLUS

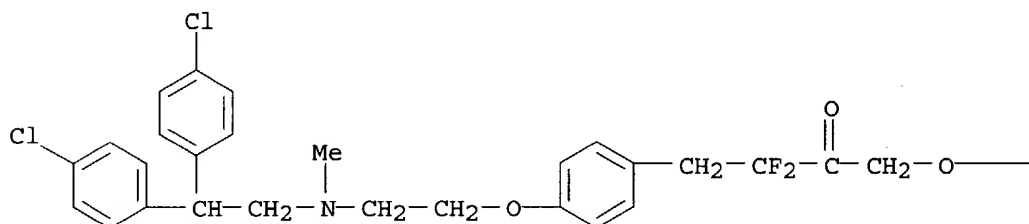
CN 2-Butanone, 4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phen  
yl]-3,3-difluoro-1-methoxy-, hydrochloride (9CI) (CA INDEX NAME)



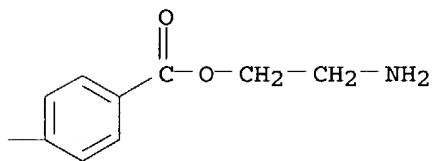
● HCl

RN 405553-05-1 HCAPLUS  
 CN Benzoic acid, 4-[4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-3,3-difluoro-2-oxobutoxy]-, 2-aminoethyl ester (9CI) (CA INDEX NAME)

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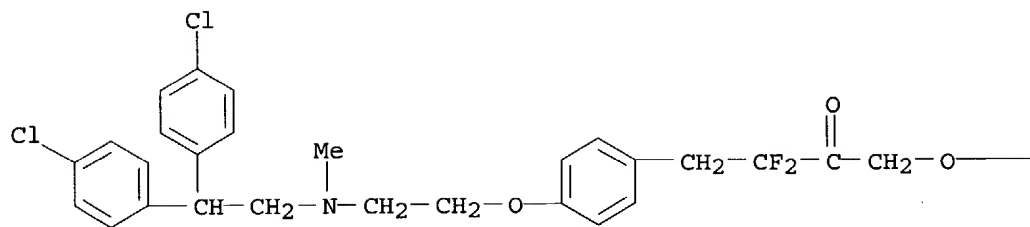


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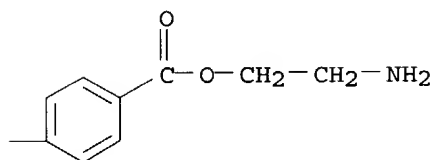
RN 405553-06-2 HCAPLUS  
 CN Benzoic acid, 4-[4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-3,3-difluoro-2-oxobutoxy]-, 2-aminoethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

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● 2 HCl

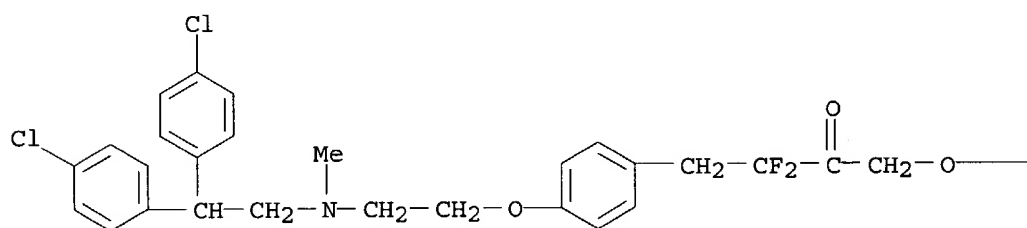
PAGE 1-B



RN 405553-09-5 HCAPLUS

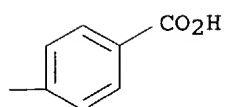
CN Benzoic acid, 4-[4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-3,3-difluoro-2-oxobutoxy]-, hydrochloride (9CI) (CA INDEX NAME)

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● HCl

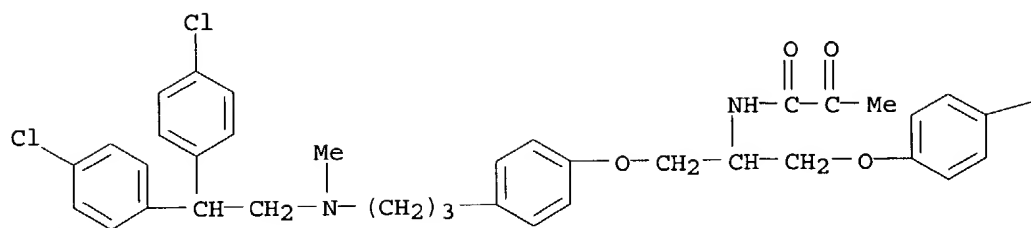
PAGE 1-B



RN 405553-11-9 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-[(1,2-dioxopropyl)amino]propoxy]- (9CI) (CA INDEX NAME)

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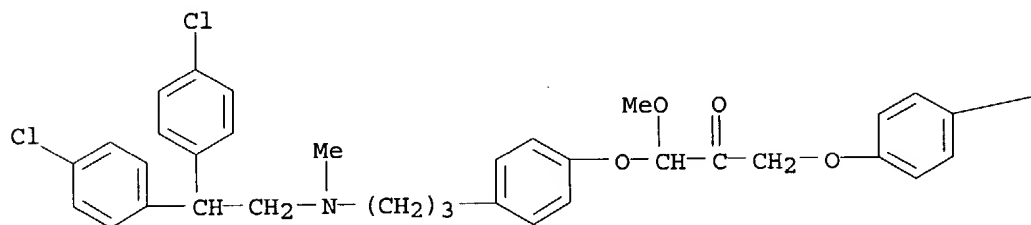


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—CO<sub>2</sub>H

RN 405553-12-0 HCAPLUS  
 CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-3-methoxy-2-oxopropoxy]-(9CI) (CA INDEX NAME)

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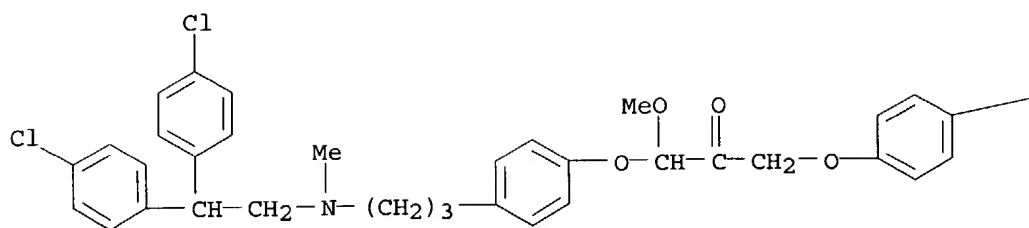
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RN 405553-13-1 HCAPLUS  
 CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-3-methoxy-2-oxopropoxy]-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 405553-12-0  
 CMF C35 H35 Cl2 N O6

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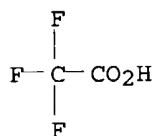
PAGE 1-B

—CO<sub>2</sub>H

CM 2

CRN 76-05-1

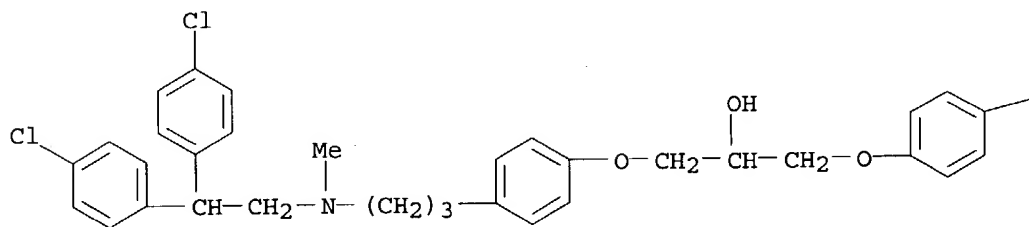
CMF C2 H F3 O2



RN 405553-14-2 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl  
phenoxy]-2-hydroxypropoxy]-, hydrochloride (9CI) (CA INDEX NAME)

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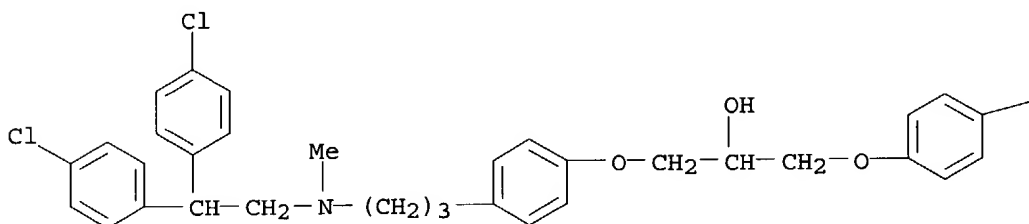
● HCl

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—CO<sub>2</sub>H

RN 405553-15-3 HCAPLUS  
 CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl  
 ]phenoxy]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

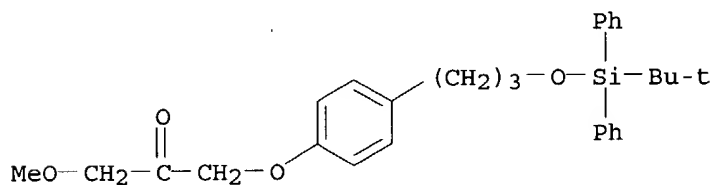
PAGE 1-A



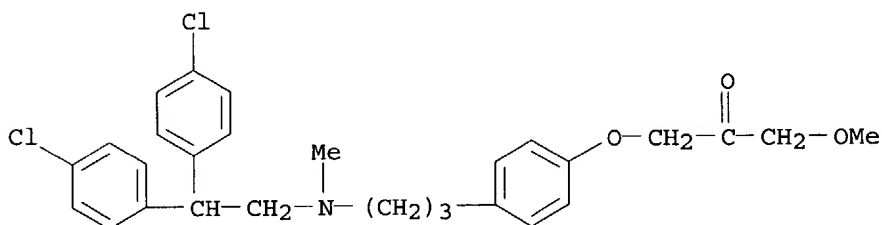
PAGE 1-B

—CO<sub>2</sub>H

RN 405553-17-5 HCAPLUS  
 CN 2-Propanone, 1-[4-[3-[[[1,1-dimethylethyl]diphenylsilyl]oxy]propyl]phenoxy  
 ]-3-methoxy- (9CI) (CA INDEX NAME)



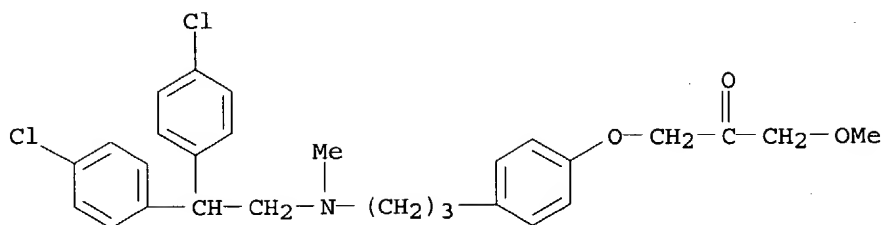
RN 405553-19-7 HCAPLUS  
 CN 2-Propanone, 1-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phe  
 noxy]-3-methoxy-, hydrochloride (9CI) (CA INDEX NAME)



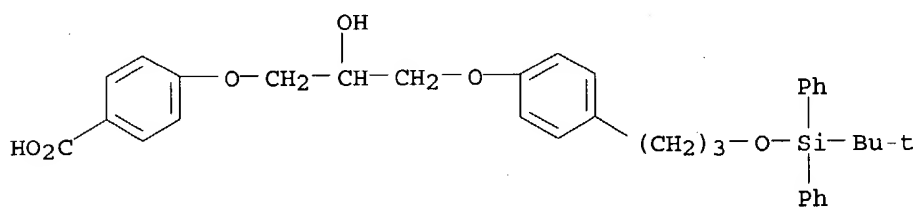
● HCl

RN 405553-20-0 HCAPLUS  
 CN 2-Propanone, 1-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phe  
 noxy]-3-methoxy- (9CI) (CA INDEX NAME)

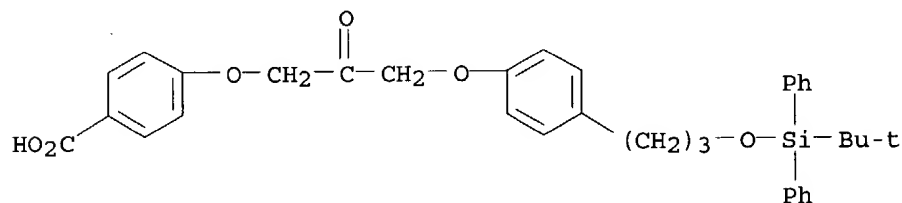




RN 405553-21-1 HCAPLUS  
 CN Benzoic acid, 4-[3-[4-[3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]propyl]phenoxy]-2-hydroxypropoxy]-(9CI) (CA INDEX NAME)

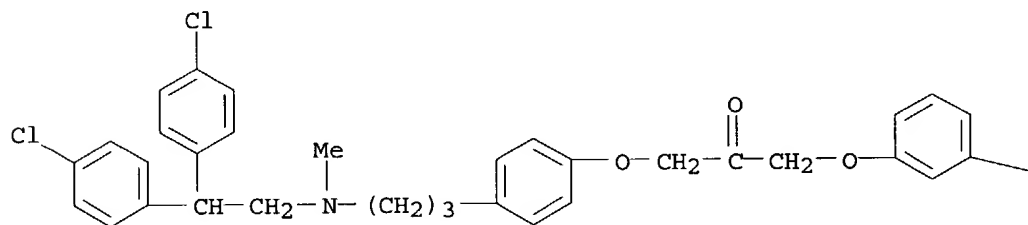


RN 405553-22-2 HCAPLUS  
 CN Benzoic acid, 4-[3-[4-[3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]propyl]phenoxy]-2-oxopropoxy]-(9CI) (CA INDEX NAME)



RN 405553-23-3 HCAPLUS  
 CN Benzoic acid, 3-[3-[4-[3-[[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-oxopropoxy]-(9CI) (CA INDEX NAME)

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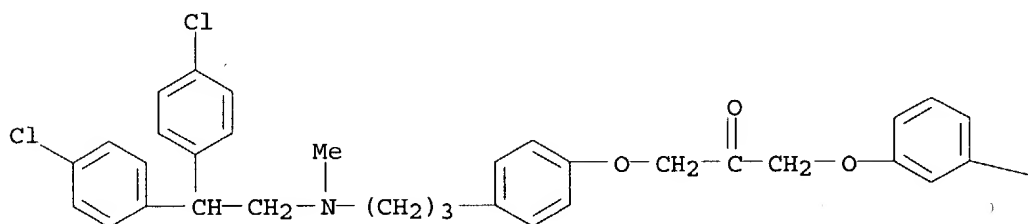
PAGE 1-B

—CO<sub>2</sub>H

RN 405553-24-4 HCAPLUS

CN Benzoic acid, 3-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-oxopropoxy]-, hydrochloride (9CI) (CA INDEX NAME)

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● HCl

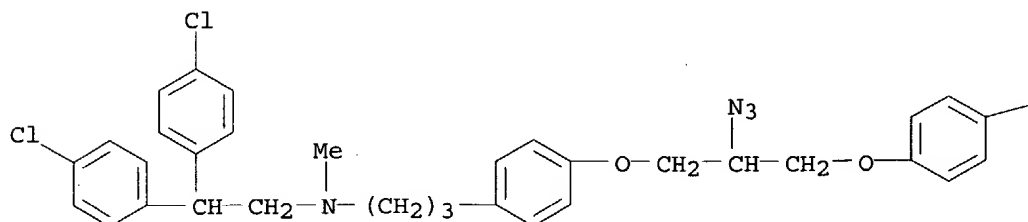
PAGE 1-B

—CO<sub>2</sub>H

RN 405553-25-5 HCAPLUS

CN Benzoic acid, 4-[2-azido-3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]propoxy]- (9CI) (CA INDEX NAME)

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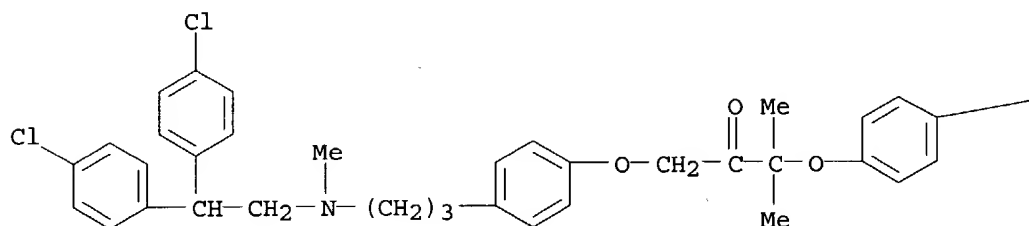
PAGE 1-B

—CO<sub>2</sub>H

RN 405553-26-6 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl  
]phenoxy]-1,1-dimethyl-2-oxopropoxy] - (9CI) (CA INDEX NAME)

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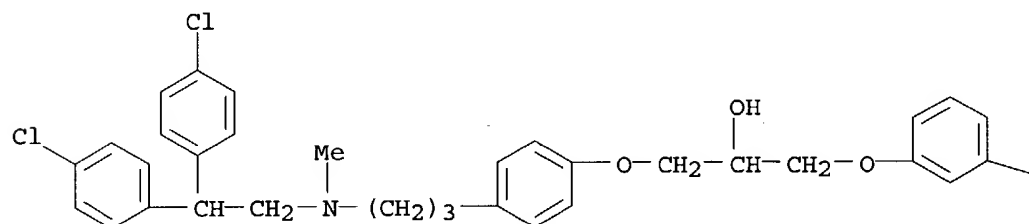
PAGE 1-B

—CO<sub>2</sub>H

RN 405553-27-7 HCAPLUS

CN Benzoic acid, 3-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl  
]phenoxy]-2-hydroxypropoxy] - (9CI) (CA INDEX NAME)

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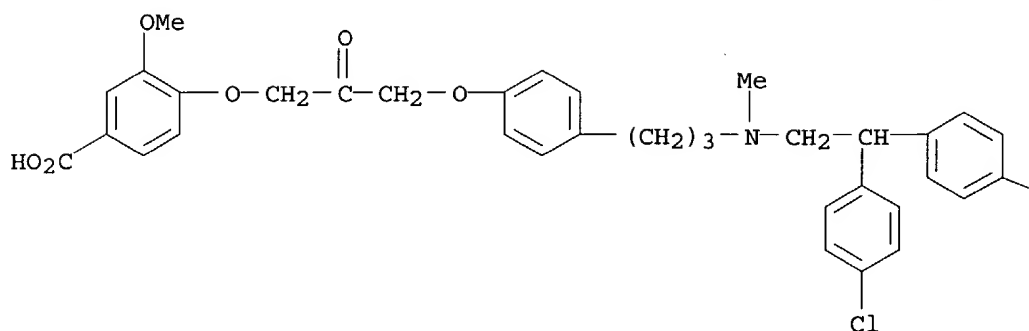
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RN 405553-28-8 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl

[phenoxy]-2-oxopropoxy]-3-methoxy- (9CI) (CA INDEX NAME)

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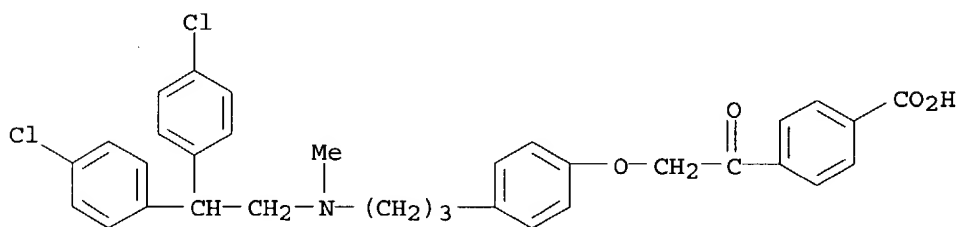


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-Cl

RN 405553-29-9 HCAPLUS

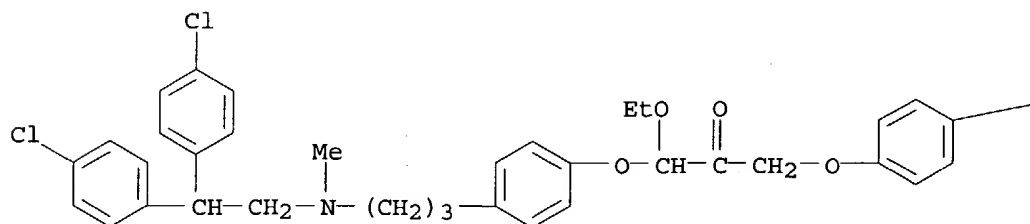
CN Benzoic acid, 4-[[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]acetyl]- (9CI) (CA INDEX NAME)



RN 405553-31-3 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-3-ethoxy-2-oxopropoxy]- (9CI) (CA INDEX NAME)

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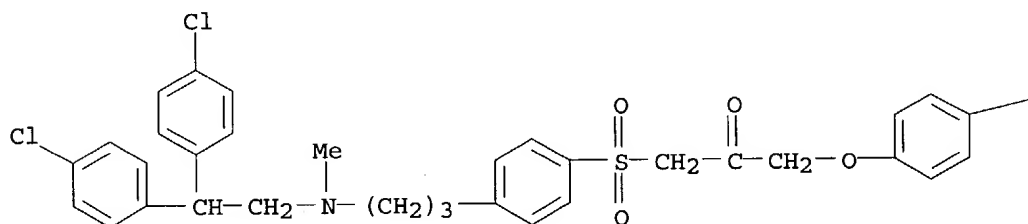
PAGE 1-B

—CO<sub>2</sub>H

RN 405553-32-4 HCAPLUS

CN Benzoic acid, 4-[3-[[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenyl]sulfonyl]-2-oxopropoxy]-(9CI) (CA INDEX NAME)

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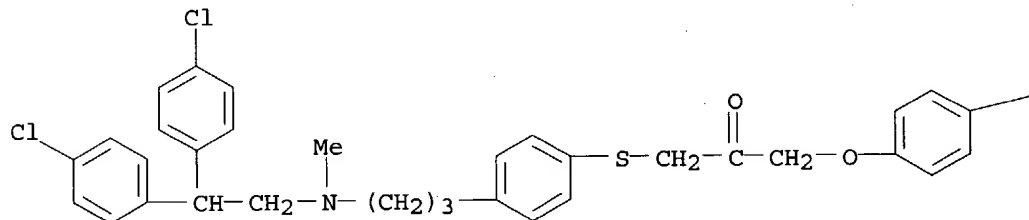
PAGE 1-B

—CO<sub>2</sub>H

RN 405553-33-5 HCAPLUS

CN Benzoic acid, 4-[3-[[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenyl]thio]-2-oxopropoxy]-(9CI) (CA INDEX NAME)

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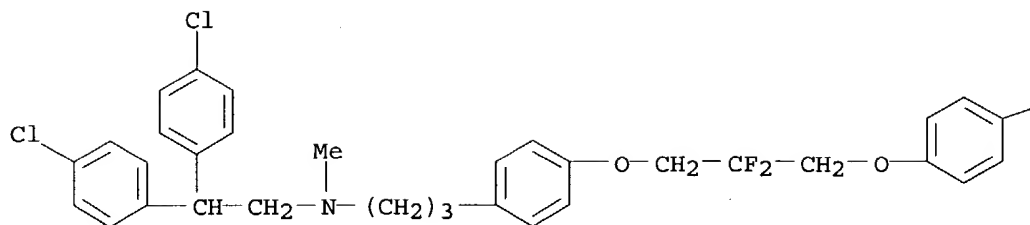
PAGE 1-B

—CO<sub>2</sub>H

RN 405553-34-6 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2,2-difluoropropoxy]-(9CI) (CA INDEX NAME)

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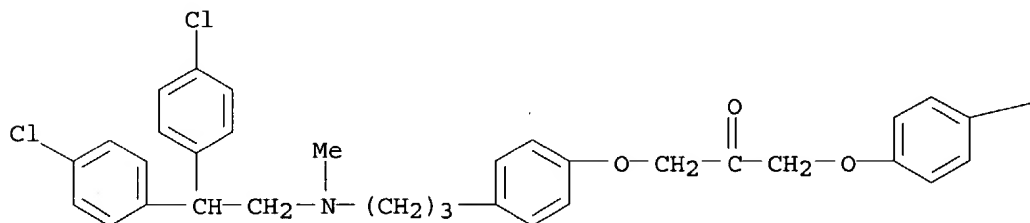
PAGE 1-B

—CO<sub>2</sub>H

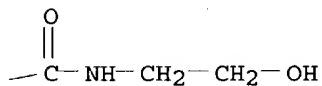
RN 405553-35-7 HCAPLUS

CN Benzamide, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2-oxopropoxy]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

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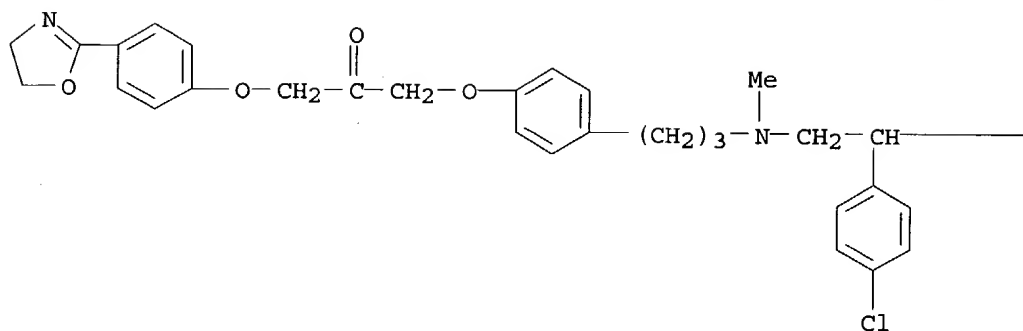
PAGE 1-B



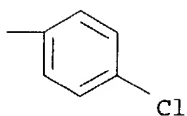
RN 405553-36-8 HCAPLUS

CN 2-Propanone, 1-[4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-3-[4-(4,5-dihydro-2-oxazolyl)phenoxy]-2-oxopropoxy]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

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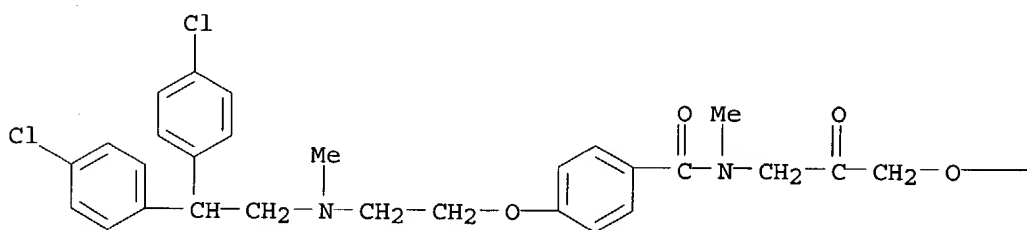


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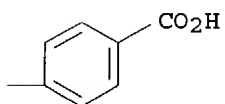


RN 405553-37-9 HCAPLUS  
 CN Benzoic acid, 4-[3-[[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]benzoyl]methylamino]-2-oxopropoxy]-(9CI) (CA INDEX NAME)

PAGE 1-A

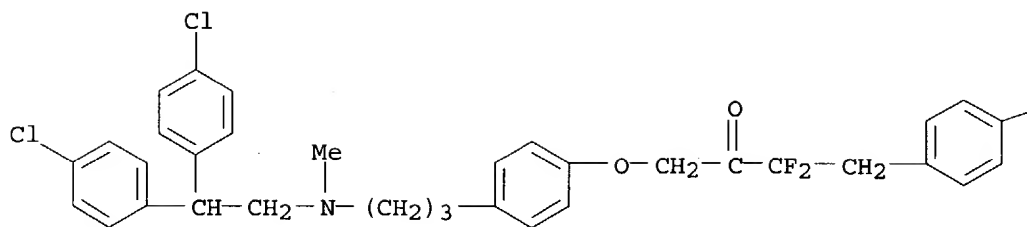


PAGE 1-B



RN 405553-38-0 HCAPLUS  
 CN Benzoic acid, 4-[4-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-2,2-difluoro-3-oxobutyl]-(9CI) (CA INDEX NAME)

PAGE 1-A

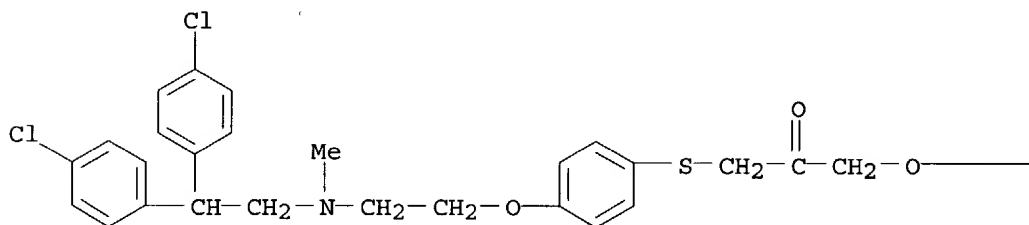


PAGE 1-B

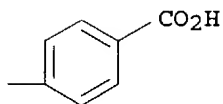
RN 405553-39-1 HCAPLUS

CN Benzoic acid, 4-[3-[[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]thio]-2-oxopropoxy]-(9CI) (CA INDEX NAME)

PAGE 1-A

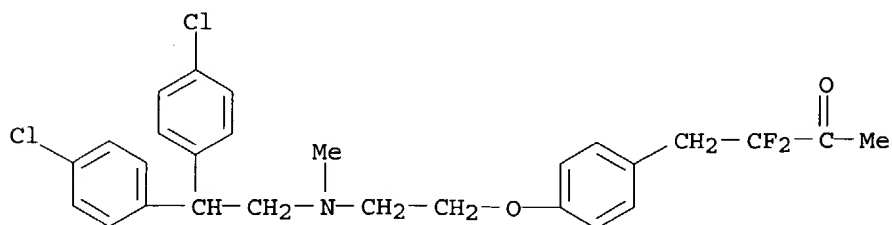


PAGE 1-B



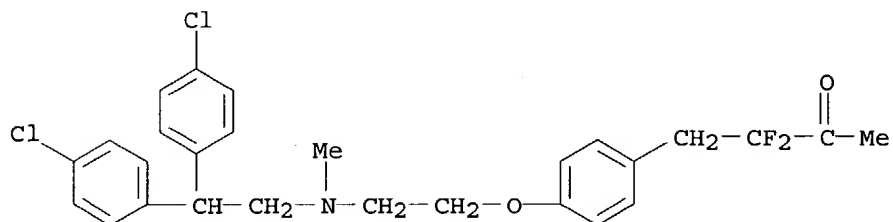
RN 405553-40-4 HCAPLUS

CN 2-Butanone, 4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-3,3-difluoro-(9CI) (CA INDEX NAME)



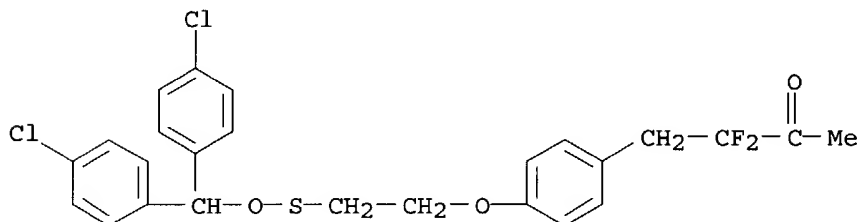


RN 405553-41-5 HCAPLUS  
 CN 2-Butanone, 4-[4-[2-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]ethoxy]phenyl]-3,3-difluoro-, hydrochloride (9CI) (CA INDEX NAME)



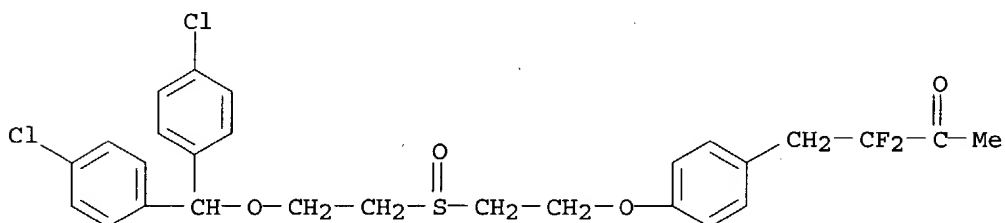
● HCl

RN 405553-42-6 HCAPLUS  
 CN Ethanesulfenic acid, 2-[4-(2,2-difluoro-3-oxobutyl)phenoxy]-, bis(4-chlorophenyl)methyl ester, compd. with hydrochloric acid (9CI) (CA INDEX NAME)

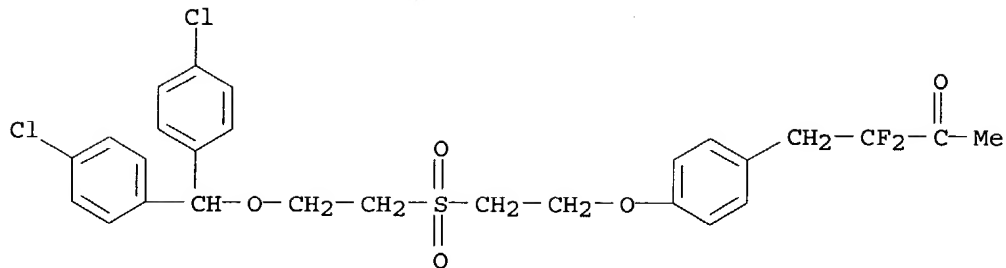


● HCl

RN 405553-43-7 HCAPLUS  
 CN 2-Butanone, 4-[4-[2-[[2-[bis(4-chlorophenyl)methoxy]ethyl]sulfinyl]ethoxy]phenyl]-3,3-difluoro- (9CI) (CA INDEX NAME)

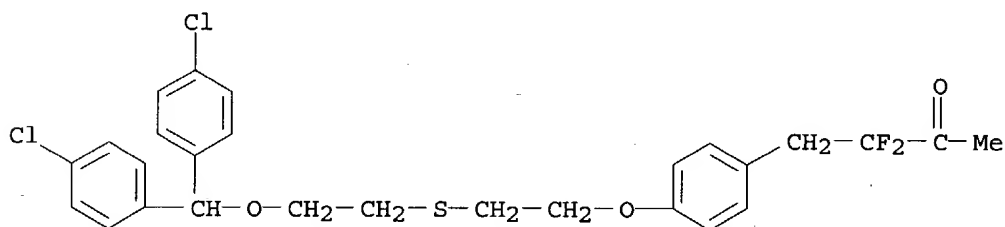


RN 405553-44-8 HCAPLUS  
 CN 2-Butanone, 4-[4-[2-[[2-[bis(4-chlorophenyl)methoxy]ethyl]sulfonyl]ethoxy]phenyl]-3,3-difluoro- (9CI) (CA INDEX NAME)



RN 405553-45-9 HCAPLUS

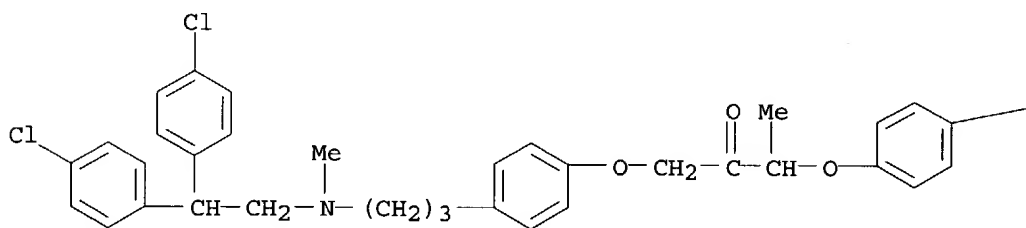
CN 2-Butanone, 4-[4-[2-[[2-[bis(4-chlorophenyl)methoxy]ethyl]thio]ethoxy]phenyl]-3,3-difluoro- (9CI) (CA INDEX NAME)



RN 405554-14-5 HCAPLUS

CN Benzoic acid, 4-[3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-1-methyl-2-oxopropoxy]-, hydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



● HCl

PAGE 1-B

-CO<sub>2</sub>H

=&gt; =&gt; d bib abs hitstr retable

DN 136:200011  
 TI Preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors  
 IN Banville, Jacques; Gai, Yonghua; Johnson, Graham; Zusi, Fred  
 Christopher; Burke, James R.  
 PA Bristol-Myers Squibb Company, USA  
 SO U.S., 112 pp., Cont.-in-part of U.S. 6,255,496.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6350892	B1	20020226	US 2000-507782	20000218
	ZA 9808687	A	20000323	ZA 1998-8687	19980922
	US 6255496	B1	20010703	US 1999-300111	19990427
PRAI	US 1997-59597P	P	19970923		
	US 1997-63518P	P	19971027		
	US 1998-151002	B1	19980910		
	US 1999-300111	A2	19990427		
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GI					

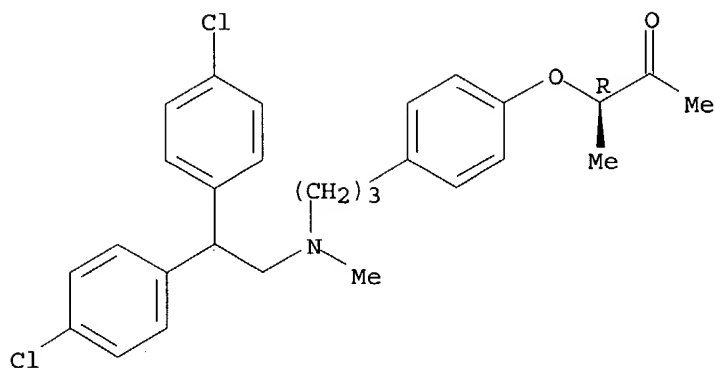
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [R5 = alk(en/yn)yl, alkoxy, alkylthio, halo, hydroxy, etc.; p = 0-2; V1 = O, S0-2, NHC:O, C:ONH; R3-4 = H, Me; R1-2 = when taken together form an oxo group or R1-2 = H, OH; Y1 = O, S0-2, aza, etc.] were prepared E.g., 4-(3-hydroxypropyl)phenol was converted to Me [4-(3-methanesulfonyloxypropyl)phenoxy]acetate in 4 steps. This intermediate was reacted with N-methyl-2,2-[di(4-chlorophenyl)]ethylamine (CH3CN, NaI, 80°C, 18 h) to give the corresponding tertiary amine. The amine was treated with trifluoromethyltrimethylsilane (PhMe, -55°C) to give isolated acetal II. Hydrolysis of II (THF, HClaq) provided the example compound trifluoromethylketone isolated as the hydrochloride. Compds. I, presented in examples, showed IC50 of 1-50 µM against cPLA2.

IT 400838-57-5P 400838-58-6P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (drug; preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)

RN 400838-57-5 HCAPLUS  
 CN 2-Butanone, 3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylaminolpropyl]phenoxy]-, (3R)- (9CI) (CA INDEX NAME)

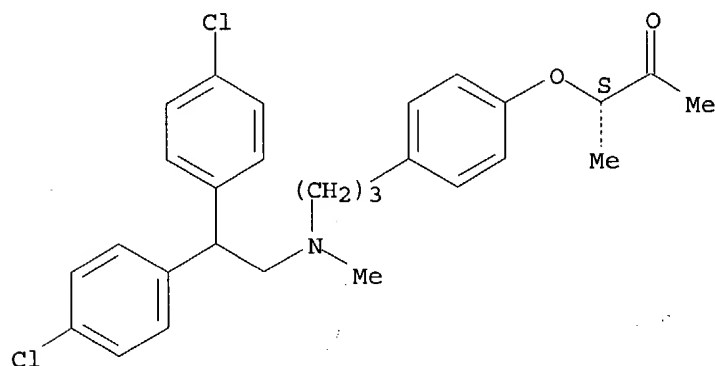
Absolute stereochemistry.



RN 400838-58-6 HCAPLUS

CN 2-Butanone, 3-[4-[3-[[2,2-bis(4-chlorophenyl)ethyl]methylamino]propyl]phenoxy]-, (3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



## RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
===== Anon	1997			JP 9268153	
Anon	1998			WO 9825893	HCAPLUS
Banville	2001			US 6255496 B1	HCAPLUS
Brickl	1980			US 4229479 A	HCAPLUS
Clemens	1995			US 5478857 A	HCAPLUS
Perrier	1995			US 5453443 A	HCAPLUS

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

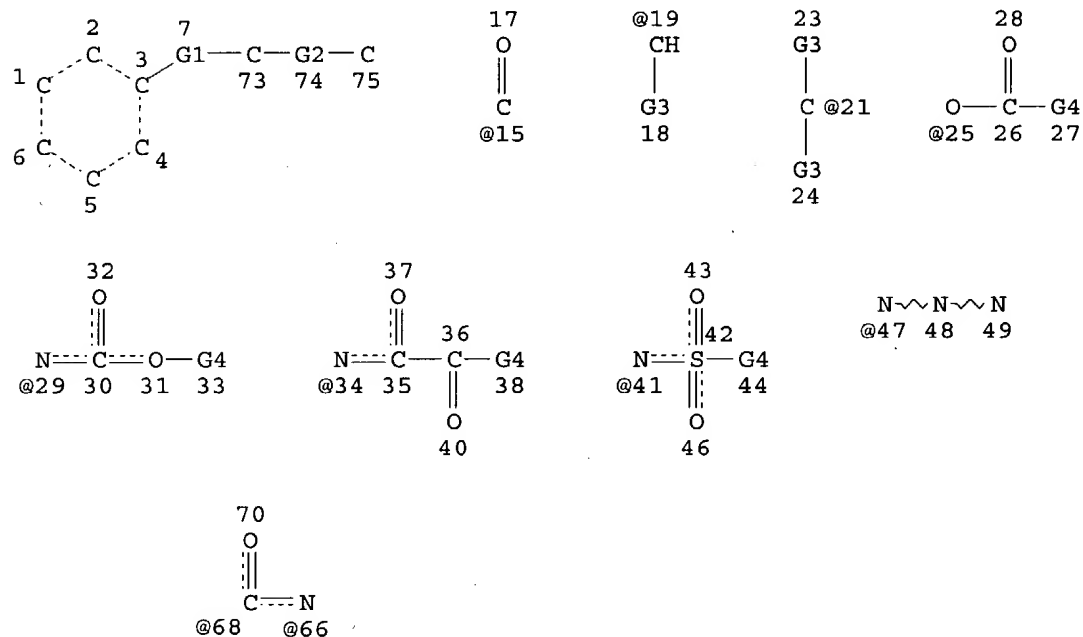
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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L6      41256 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?PHOSPHOLIPASE?
L7      4312 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PLA2
L8      42502 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L5 OR L6 OR L7)
L9      35483 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND (PD<=20000511 OR
PRD<=20000511 OR AD<=20000511)
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L9 OR L9
L13     5000 SEA FILE=HCAPLUS RAN=(1994:260855,1996:496207) ABB=ON  PLU=ON
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L9 OR L9
L16     5000 SEA FILE=HCAPLUS RAN=(1981:456771,1988:88252) ABB=ON  PLU=ON
L9 OR L9
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L31     52427 SEA FILE=REGISTRY ABB=ON  PLU=ON  L30
L32     1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "PHOSPHOLIPASE A2"/CN
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L34     105 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PLA 2 OR PL A2
L35     1711 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PHOSPHOLIPIN OR SUPERBIN OR
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E OR NIGROXIN OR LECITHINASE OR LECITASE OR ACANTHOXIN OR
AGELOTOXIN OR AMMODYTOXIN OR CONODIPINE OR (EC OR "E C") (W) 3 1
1 4
L36     581 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L33 OR L34 OR L35) NOT L8
L37     SEL  PLU=ON  L36 1- RN :      591 TERMS
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L39     7019 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 NOT (L9 OR L36)
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L42     3519 SEA FILE=HCAPLUS RAN=(,2002:851704) ABB=ON  PLU=ON  L39 OR L39
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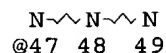
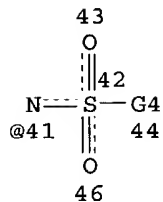
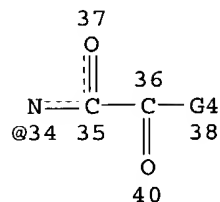
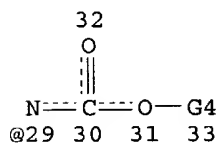
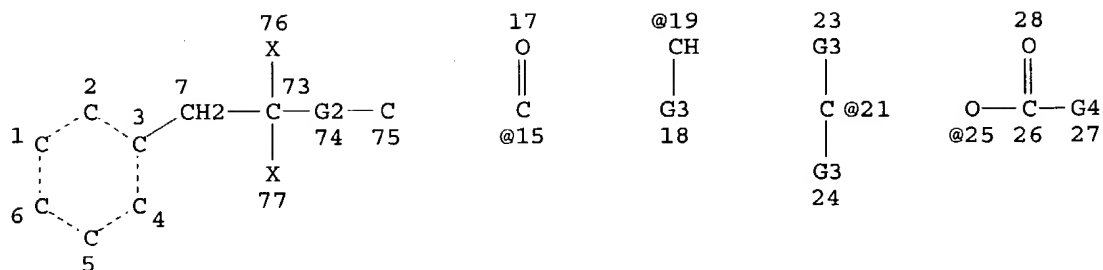
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 L46 51797 SEA FILE=REGISTRY ABB=ON PLU=ON L45  
 L47 2500 SEA FILE=HCAPLUS RAN=(2000:32864,) ABB=ON PLU=ON L9 OR L9  
 L49 SEL PLU=ON L47 1- RN : 52427 TERMS (TERM LIMIT EXCEE  
 DED)  
 L50 52427 SEA FILE=REGISTRY ABB=ON PLU=ON L49  
 L63 212172 SEA FILE=REGISTRY ABB=ON PLU=ON (L19 OR L21 OR L23 OR L25 OR  
 L27 OR L29 OR L31 OR L38 OR L44 OR L46 OR L50)  
 L65 STR



VAR G1=CH2/O/S/N/68-3 66-73  
 VAR G2=15/CH2/19/21  
 VAR G3=OH/25/NH2/47/29/34/41/X  
 VAR G4=AK/CB  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 1  
 NUMBER OF NODES IS 43

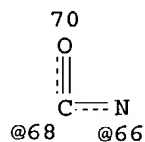
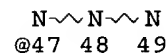
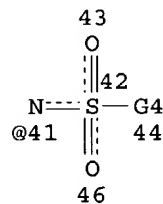
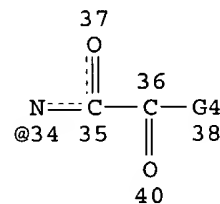
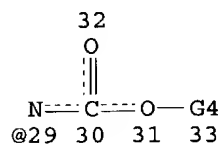
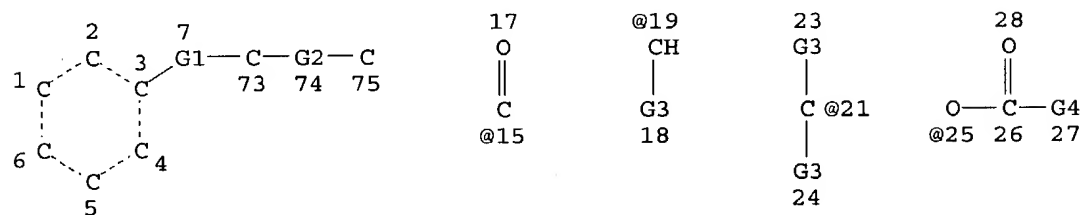
STEREO ATTRIBUTES: NONE  
 L66 3931 SEA FILE=REGISTRY SUB=L63 SSS FUL L65  
 L67 STR



VAR G2=15/CH2/19/21  
 VAR G3=OH/25/NH2/47/29/34/41/X  
 VAR G4=AK/CB  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 1  
 NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE  
 L69 15 SEA FILE=REGISTRY SUB=L66 SSS FUL L67  
 L70 STR



VAR G1=O/S/N/68-3 66-73  
 VAR G2=15/CH2/19/21  
 VAR G3=OH/25/NH2/47/29/34/41/X

VAR G4=AK/CB

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

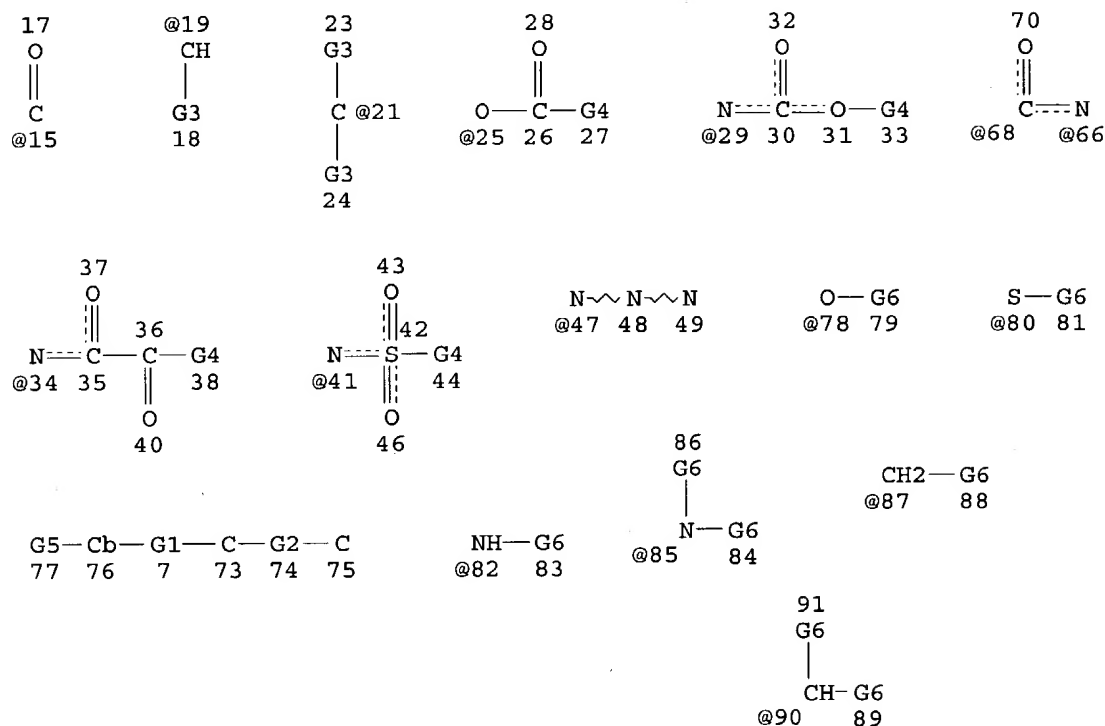
RSPEC 1

NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE

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L73 STR



VAR G1=CH2/O/S/N/68-76 66-73

VAR G2=15/CH2/19/21

VAR G3=OH/25/NH2/47/29/34/41/X

VAR G4=AK/CB

VAR G5=78/80/82/85/87/90

VAR G6=AK/CB

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 76

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 53

STEREO ATTRIBUTES: NONE

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L76 1498 SEA FILE=REGISTRY SUB=L74 SSS FUL L73

100.0% PROCESSED 2356 ITERATIONS  
SEARCH TIME: 00.00.01

1498 ANSWERS



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L3 50 S L2  
L4 2733 S ?PHOSPHOLIPASE?/CNS

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L5 29567 S L4  
L6 41256 S ?PHOSPHOLIPASE?  
L7 4312 S PLA2  
L8 42502 S L5-L7  
L9 35483 S L8 AND (PD<=20000511 OR PRD<=20000511 OR AD<=20000511)  
L10 35483 S L9 OR L9  
L11 5000 S L10 RAN=(1998:711656,)  
L12 5000 S L10 RAN=(1996:496210,1998:711544)  
L13 5000 S L10 RAN=(1994:260855,1996:496207)  
L14 5000 S L10 RAN=(1991:512049,1994:260585)  
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L19 3343 S L18  
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L21 7429 S L20

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L22 SEL L15 1- RN : 8249 TERMS  
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L23 8249 S L22

FILE 'HCAPLUS' ENTERED AT 14:19:36 ON 24 JUN 2004

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L24 SEL L14 1- RN : 8522 TERMS  
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L25 8521 S L24

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SET SMARTSELECT ON  
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L27 16081 S L26

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L28 SEL L12 1- RN : 33965 TERMS  
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L29 33965 S L28

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L30 SEL L11 1- RN : 52427 TERMS  
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L31 52427 S L30  
E PHOSPHOLIPASE A2/CN  
L32 1 S E3

FILE 'HCAPLUS' ENTERED AT 14:33:49 ON 24 JUN 2004  
L33 13318 S L32  
L34 105 S PLA 2 OR PL A2  
L35 1711 S PHOSPHOLIPIN OR SUPERBIN OR PHOSPHATIDOLIPASE OR PHOSPHATIDE  
L36 581 S L33-L35 NOT L8

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L38 591 S L37

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L39 7019 S L8 NOT L9,L36  
L40 7019 S L39 OR L39  
L41 3500 S L40 RAN=(2002:851707,)  
L42 3519 S L40 RAN=(,2002:851704)

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L45 SEL L42 1- RN : 51797 TERMS  
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L46 FILE 'REGISTRY' ENTERED AT 14:44:40 ON 24 JUN 2004  
51797 S L45

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L52 1 S US20020037875/PN OR US2000-203741#/AP,PRN  
E BANVILLE J/AU  
L53 32 S E3,E4  
E REMILLARD R/AU  
L54 55 S E3-E5,E8  
E BALASUBRAMANIAN N/AU  
L55 235 S E3-E7,E15,E16  
E BOUTHILLIER G/AU  
L56 6 S E4  
E MARTEL A/AU  
L57 124 S E3-E15  
L58 431 S L52-L57  
L59 105 S L51 AND BENZEN?/SC,SX  
L60 531 S L58,L59

FILE 'REGISTRY' ENTERED AT 14:54:09 ON 24 JUN 2004

FILE 'HCAPLUS' ENTERED AT 14:54:09 ON 24 JUN 2004  
SET SMARTSELECT ON  
L61 SEL L60 1- RN : 14545 TERMS  
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 14:54:31 ON 24 JUN 2004  
L62 14545 S L61  
L63 212172 S L19,L21,L23,L25,L27,L29,L31,L38,L44,L46,L50  
L64 50 S L2 SAM SUB=L63  
L65 STR L2  
L66 3931 S L65 FUL SUB=L63  
SAV L66 KUMAR848/A  
L67 STR L65  
L68 1 S L67 SAM SUB=L66  
L69 15 S L67 FUL SUB=L66  
SAV L69 KUMAR848A/A  
L70 STR L65  
L71 50 S L70 SAM SUB=L66  
L72 2348 S L70 FUL SUB=L66  
SAV L72 KUMAR848B/A  
L73 STR L65  
L74 2356 S L69,L72  
L75 50 S L73 SAM SUB=L74  
L76 1498 S L73 FUL SUB=L74  
SAV L76 KUMAR848C/A  
L77 STR L65  
L78 4 S L77 SAM SUB=L75

L79 4 S L77 FUL SUB=L75

FILE 'HCAPLUS' ENTERED AT 15:08:50 ON 24 JUN 2004

L80 35012 S L76  
L81 1 S L80 AND L52  
L82 7 S L80 AND L53-L57  
L83 7 S L81,L82  
L84 5 S L83 AND L51  
L85 178 S L80 AND L51  
L86 161 S L85 AND (PD<=20000511 OR PRD<=20000511 OR AD<=20000511)  
L87 78 S L76 (L) (THU OR PAC OR PKT OR BAC OR DMA)/RL AND L86  
L88 49 S L87 AND L33-L35  
L89 23 S L87 AND ?PLA2?  
L90 53 S L87 AND PHOSPHOLIPASE A2  
L91 54 S L88-L90  
SEL RN L52

FILE 'REGISTRY' ENTERED AT 15:51:56 ON 24 JUN 2004

L92 125 S E1-E125  
L93 81 S L66 AND L92  
L94 44 S L92 NOT L93  
L95 37 S L94 AND 46.150.18/RID

FILE 'HCAPLUS' ENTERED AT 17:16:26 ON 24 JUN 2004

L96 1 S L93

FILE 'REGISTRY' ENTERED AT 17:16:33 ON 24 JUN 2004

L97 3 S L95 AND (C33H31CL2NO4 OR C40H45CL2NO6 OR C36H37CL2NO6)

FILE 'HCAPLUS' ENTERED AT 17:20:26 ON 24 JUN 2004

L98 1 S L97  
L99 1 S L96,L98  
L100 1 S L99 AND L51-L58  
L101 53 S L91 NOT L100  
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 17:22:01 ON 24 JUN 2004

L102 647 S E126-E772  
L103 641 S L76 AND L102

FILE 'HCAPLUS' ENTERED AT 17:24:31 ON 24 JUN 2004

L104 4 S L84 NOT L100  
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 17:25:27 ON 24 JUN 2004

L105 55 S E773-E827  
L106 55 S L105 NOT L93  
L107 55 S L106 NOT L69  
L108 4 S L107 AND (C35H43CL2NO5 OR C28H31CL2NO2 OR C37H47CL2NO5)  
L109 2 S L107 AND C28H31CL2NO2

FILE 'HCAPLUS' ENTERED AT 17:29:22 ON 24 JUN 2004

L110 1 S L109  
L111 1 S L110 AND L53-L57

FILE 'REGISTRY' ENTERED AT 17:30:24 ON 24 JUN 2004

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